

PHEV and EV Battery Performance and Cost Assessment

Project Name: Core BatPaC Development and Implementation

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Organization: Argonne National Laboratory

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June 9, 2015

Project ID: ES111

Overview

Timeline

- Start: 2012
- End: 2016

Barriers

Development of a PHEV and EV batteries that meet or exceed DOE/USABC goals

A. Cost

C. Performance

Budget

- FY14: 575K
- FY15: 575K

Collaborators

- U.S. Environmental Protection Agency
- B&W MEGTEC, GM, LGChem, PPG
- 3M, Amprius, Envia

Relevance

- This modeling effort supports projects through the development and utilization of efficient simulation, analysis, and design tools for advanced lithium ion battery technologies.
- This project provides assessment of the technology developments through projections of cost and performance at the pack level
- The EPA uses BatPaC to predict the cost of battery technologies for their 2017-2025 rule making
 - Argonne updates BatPaC with cost inputs, modification of constraints, allow variable factory utilization, etc.
- BatPaC is the only peer-reviewed LIB design and cost model available in the public domain

Objectives and Approach

Objective: Develop and utilize efficient simulation and design tools for Li-ion batteries to predict:

- Precise overall and component mass and dimensions
- Cost and performance characteristics
- Battery pack values from bench-scale results

Approach: Design a battery based on power and energy requirements for a specific cell chemistry, feeding into a cost calculation that accounts for materials and processes required

- Optimized battery design to meet the specifications
- Cost based on a described manufacturing process

Approach: Reduce uncertainty in model predictions

- Update the default material and processing costs
- Develop higher fidelity models of the physical and electrochemical phenomenon, and manufacturing flow path (quantify energy needs)
- Validate results with OEMs, manufacturers, component developers

BatPaC designs the battery and calculates its mass, volume, materials, heat transfer needs, and cost

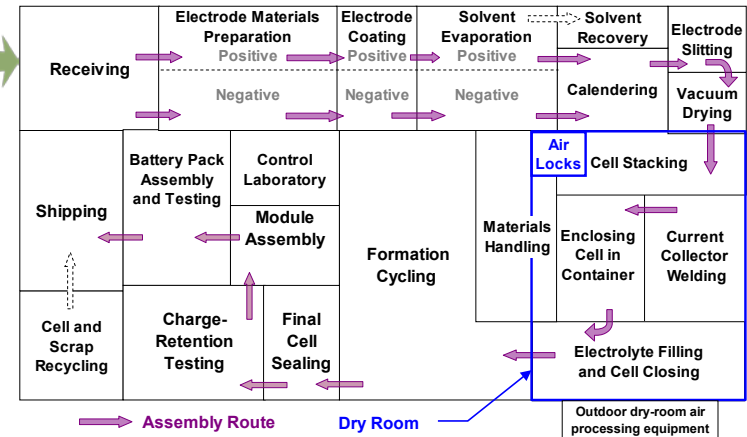
Iterate Over Governing Eqs. & Key Design Constraints

- Cell, module, & pack format
- Maximum electrode thickness
- Fraction of OCV at rated power

Battery Pack Components

- Volume
- Mass
- Materials
- Heat generation

$$\text{Process cost} = \text{Baseline cost} \cdot \left(\frac{\text{Processing rate}}{\text{Baseline processing rate}} \right)^p$$



• Pack specifications

- Power and energy (range)
- Number of cells

• Cell Chemistry

- Area-specific impedance (ASI)
- Reversible capacity C/3
- OCV as function of SOC
- Physical properties

Governing Equations

$$E = N \cdot C \cdot \left(U_E - \frac{C}{3} \frac{ASI_E}{A} \right)$$

$$L = \frac{C}{Q \cdot \rho \cdot \varepsilon \cdot A}$$

$$I = \frac{P}{A \cdot N \cdot U_p \left[\frac{V}{U} \right]}$$

$$A = \frac{ASI_p \cdot P}{N \cdot (U_p)^2 \left[\frac{V}{U} \right] \left[1 - \left[\frac{V}{U} \right] \right]}$$

$$ASI = \frac{\alpha + f(I)}{L} + \beta$$

Total Cost to OEM

- Materials & purchased items
- Individual process steps
- Overhead, depreciation, etc.
- Warranty

Technical Accomplishments and Progress

A new version (3B) of BatPaC has been released

Milestone: Release new BatPaC version, Q2-FY15.

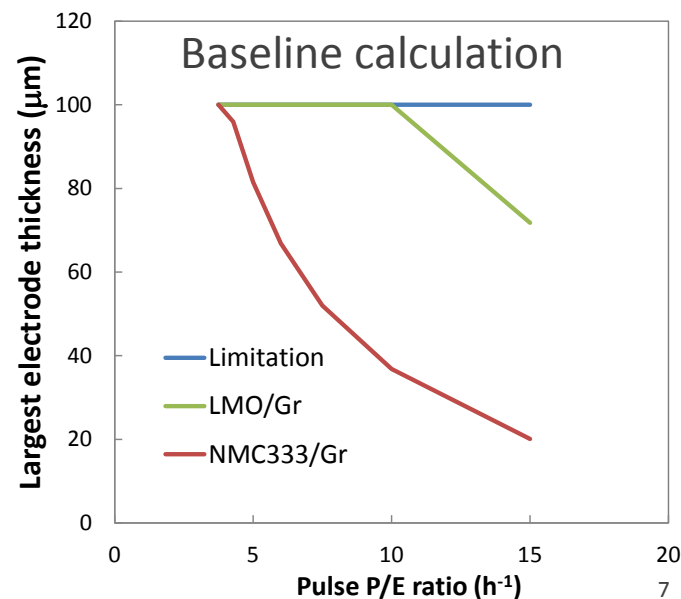
– Status: **Completed**

- Added a table of results corresponding to USABC format
 - Updated thermal management calculations
 - Provided rapid gas discharge pathway from modules
 - Reconfigured to enable cell cost calculations
- Updated costs of LFP cathode, current collectors, separator, and electrolyte
- Expect to release a newer version later this year
 - Developing understanding of uncertainties
 - Electrode thickness limitation, cathode material cost, etc.

Technical Accomplishments and Progress

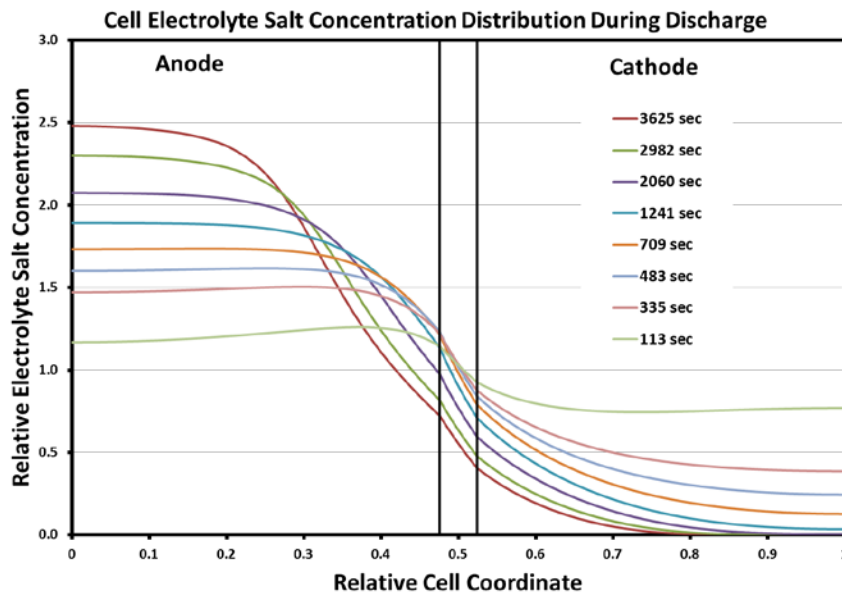
Improved optimal electrode loading calculation

- Electrode loading key design & cost uncertainty
- Higher mAh/cm² reduces cost and increases Wh/L
- Key factor to quantify benefit of new materials
- Previously set thickness to minimum of two calcs
 - Thickness needed to meet pulse power requirement
 - Maximum thickness limit (100 μm)
- New approach uses
 - Continuous power demand
 - Electrolyte transport limitations



Characteristic length for electrolyte transport key to calculating optimal electrode loading

- Concentration gradients limit utilization of electrode capacity



NCA/Graphite Li-Ion Cell Simulation
245 μm Electrodes 1C Discharge

Electrolyte Concentrated Solution
Transport Equation

$$\varepsilon \frac{\partial c}{\partial t} = \frac{\varepsilon}{\tau} \nabla \cdot (D \nabla c) + \frac{\nabla \cdot [(1 - c \bar{V}_e)(1 - t_+^o) \vec{i}_2]}{z_+ \nu_+ F}$$

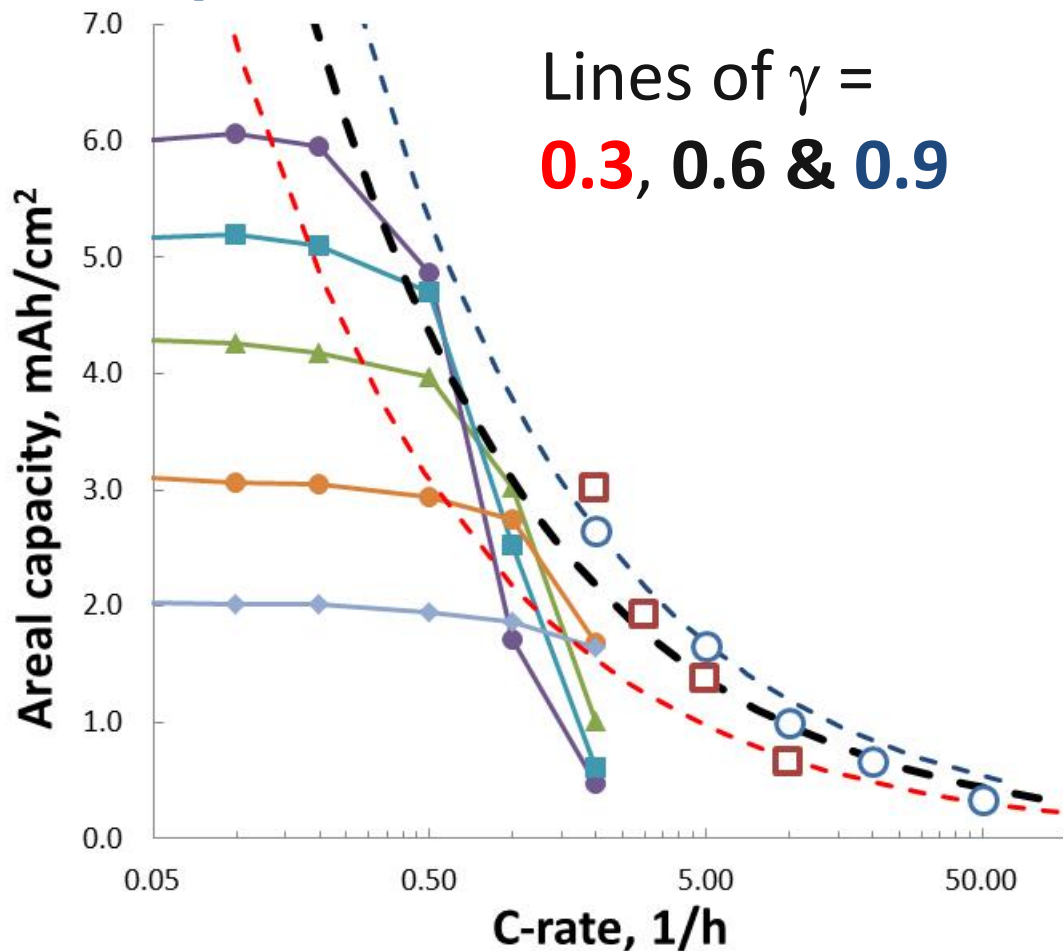
Characteristic Length, L^* , in
Porous Electrode

$$L^* = \frac{\left(\frac{\varepsilon}{\tau}\right) D c z_+ \nu_+ F}{(1 - t_+^o) I}$$

Optimal Loading as a Fraction
of Characteristic Length

$$Q_A = Q_v L = Q_v \gamma L^* = \sqrt{\frac{\gamma Q_v \left(\frac{\varepsilon}{\tau}\right) D c z_+ \nu_+ F t_d}{(1 - t_+^o)}}$$

Designing maximum electrode loading by rate required for constant discharge



Open symbols transformed from: Zheng et al *Electrochim. Acta* **71** (2012) 258 [blue LFP/Gr & red NMC333/Gr]

For these tested electrodes
NMC622/Graphite (closed symbols)

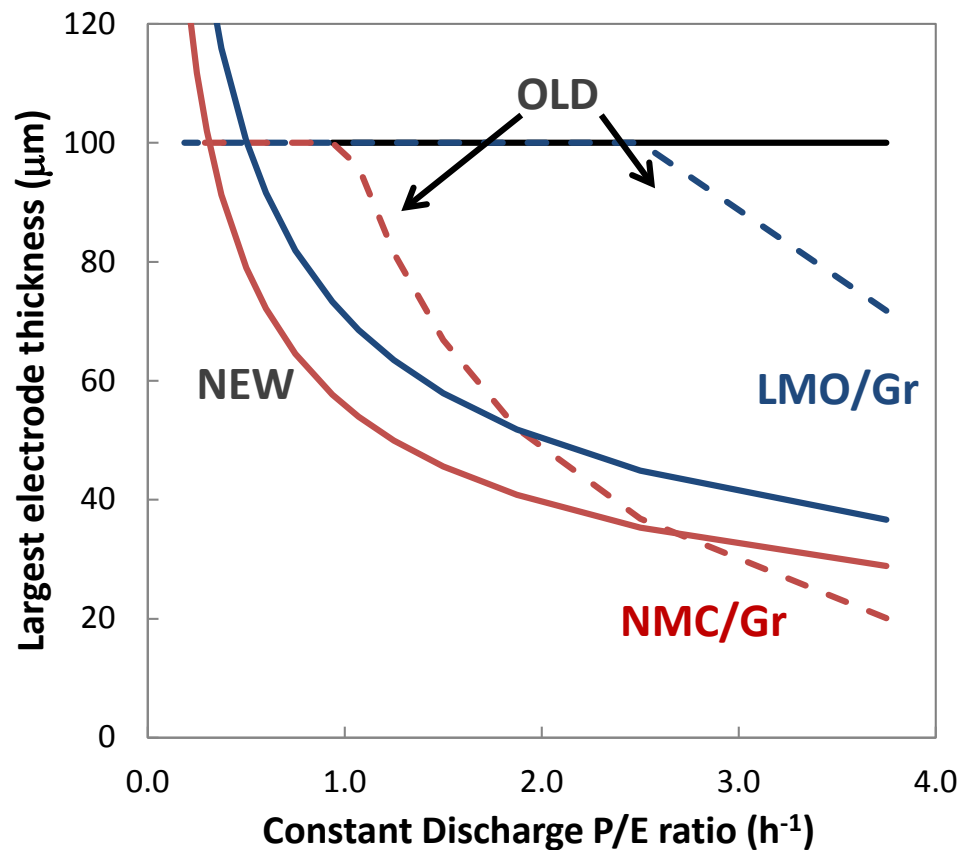
Continuous C-rate	Design capacity, mAh/cm ²
C/5	4.8
C/3	3.8
C/2	3.1
1C	2.1
2C	1.5
3C	1.25

Designs should target electrode thicknesses of $\sim 0.3L^*$ or less at required C-rate

New methodology accurately reflects transport limitations - thinner electrodes for most designs

- Thinner electrodes result in higher costs
- Higher energy density materials key path to reduce active & inactive cost contributions

$$Q_A = \sqrt{\frac{\lambda Q_v \left(\frac{\varepsilon}{\tau} \right) DcFt_d}{(1 - t_+^o)}}$$



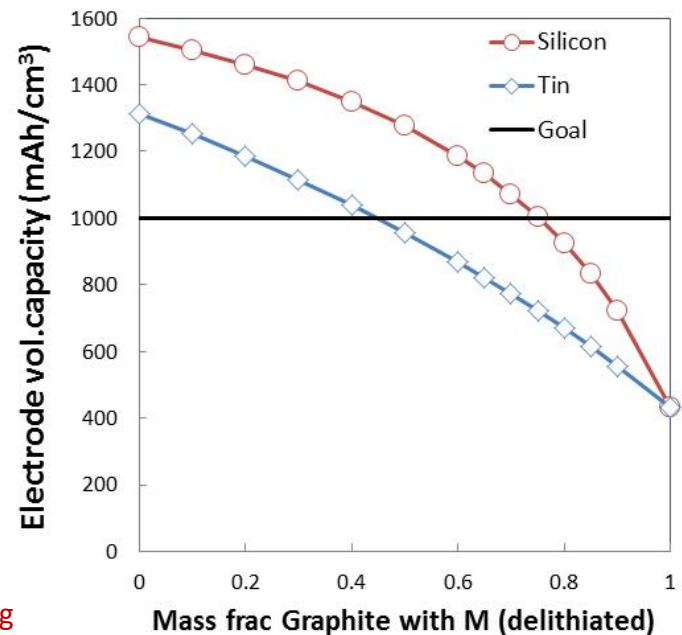
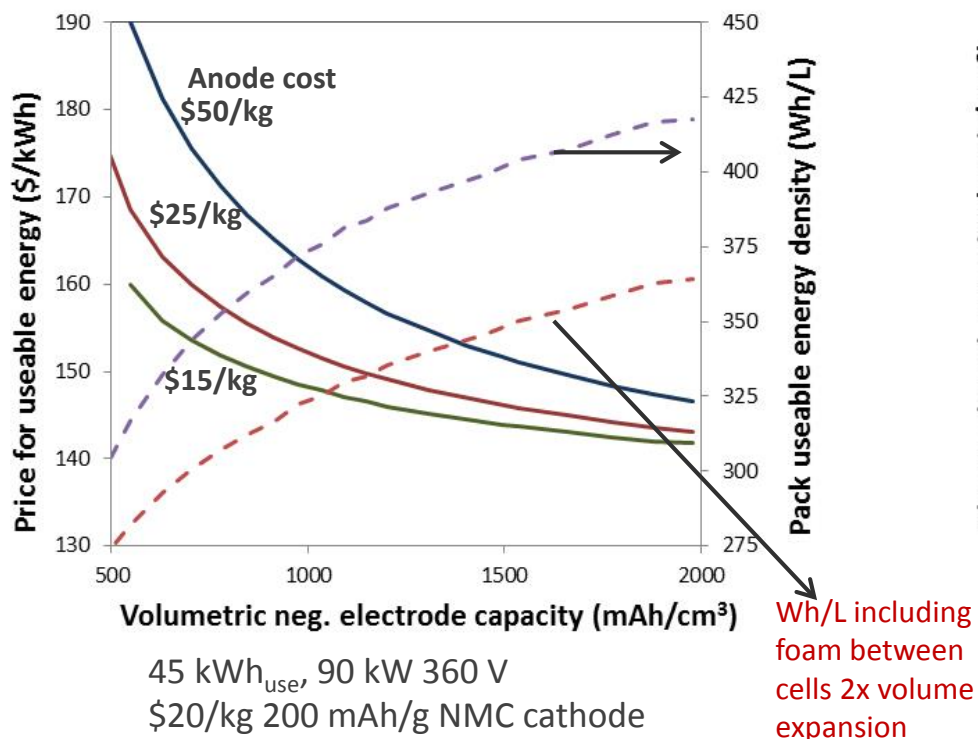
Technical Accomplishments and Progress

Material requirements to meet USABC EV targets

- Researchers require translation of pack level targets to materials level requirements
- Priority research directions require quantitative connection to real world values
- Primary focus of calculations will be on cost
 - Pack mass and volume show same trend (both decrease with decreasing cost)
 - Volume target is most challenging to meet ($500 \text{ Wh}_{\text{use}}/\text{L}$)

Advanced anodes should target $>1000 \text{ mAh/cm}^3$

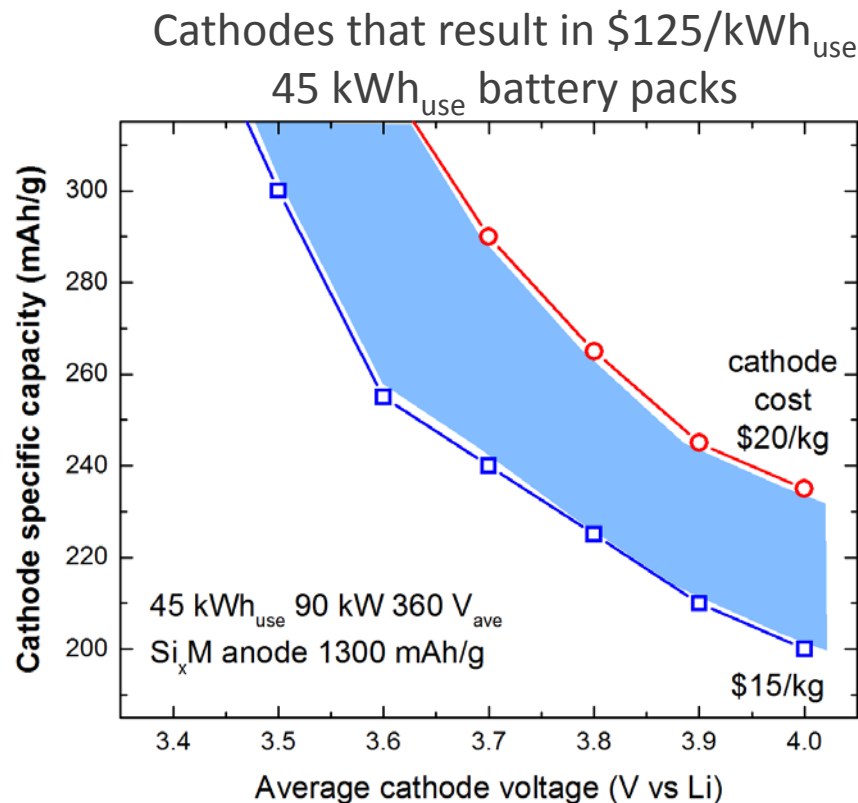
- Pack level benefits reach diminishing returns after 1000 mAh/cm^3 for both cost and energy density
 - $\text{mAh/cm}^3 = \rho \cdot \epsilon \cdot Q \left[\frac{\text{g}}{\text{cm}^3_{\text{act}}} \cdot \frac{\text{cm}^3_{\text{act}}}{\text{cm}^3_{\text{elect}}} \cdot \frac{\text{mAh}}{\text{g}} \right]$
- Silicon with $<75 \text{ wt\%}$ graphite can achieve target



Electrode volumetric capacity uses lithiated basis $\text{Li}_{4.4}\text{Si}$ or $\text{Li}_{4.4}\text{Sn}$ and maximum active material volume fraction of 65%

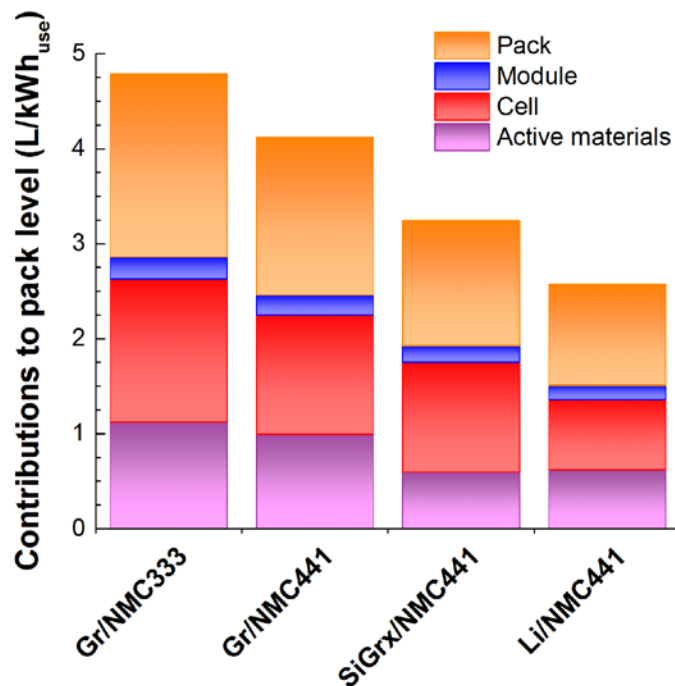
Advanced cathodes should target $>900 \text{ Wh/kg}_{\text{cath}}$

- Cathode requirements challenging to meet USABC pack level targets
- $>900 \text{ Wh/kg}_{\text{cathode}}$ (vs Li) ($>600 \text{ mAh/cm}^3$) required when paired with Si composite anode
- Material cost target is consistent with Mn-rich compositions

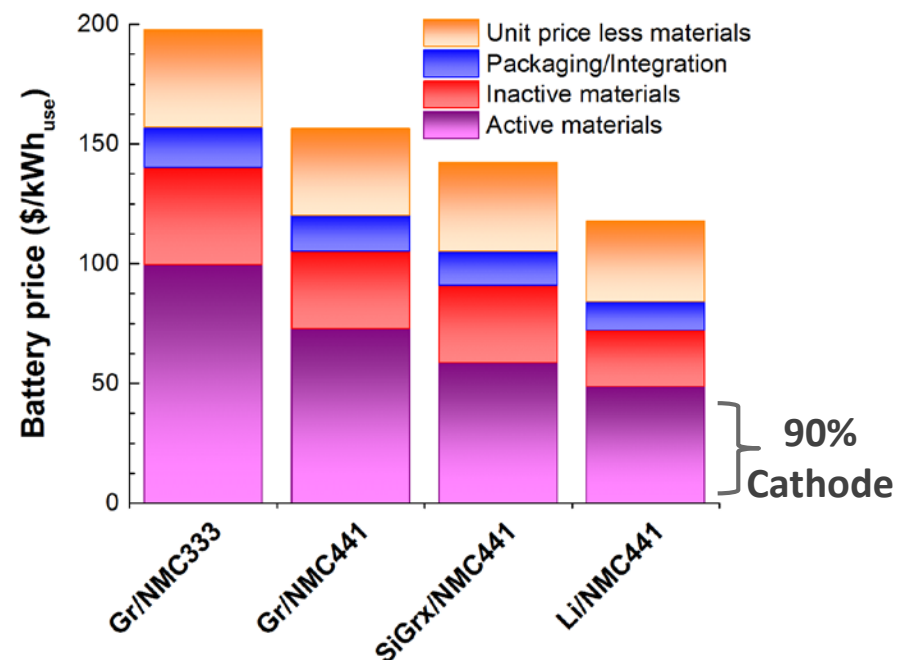


Performance gains resulting from advanced anodes and high voltage NMC cathode

- Cathode remains largest savings opportunity
- Advanced anodes save 37% volume and 25% cost



100 kWh_{use}, 80 kW, 360 V



Technical Accomplishments and Progress

Comparison with Beyond Li-ion Possibilities

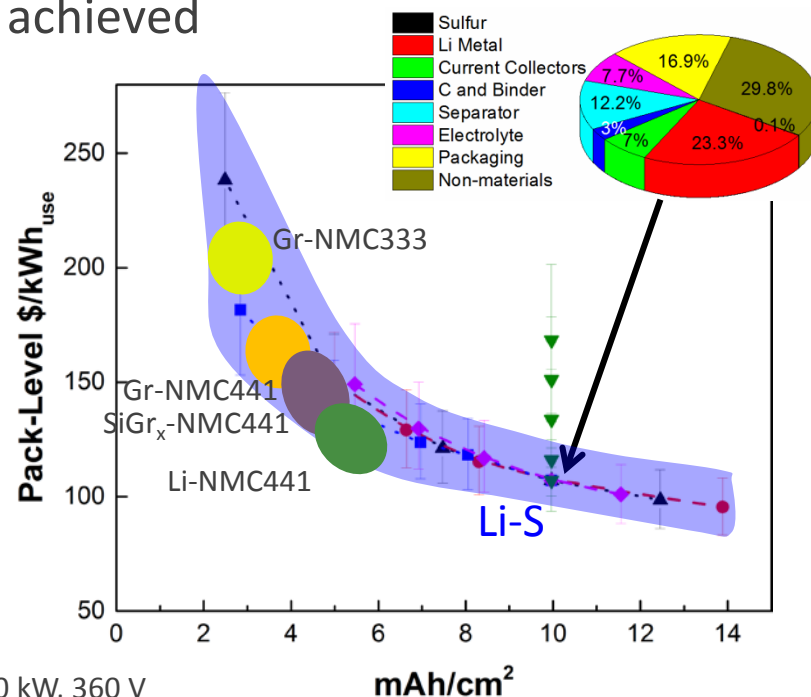
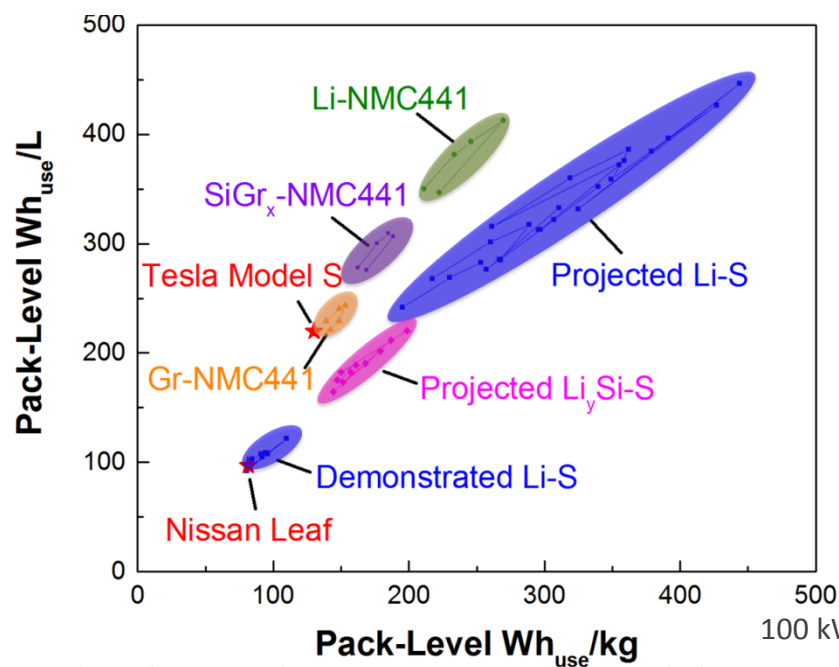
- Intercalation hosts used in Li-ion provide competitive energy densities at the expense of mass
- Successful development of Li-metal would benefit Li-ion as well as Li/S
- Li/S key challenges to be addressed
 - New electrolytes that do not require large excesses (unlike DME:DOL)
 - Reversible and stable Li-metal electrode (Li_ySi does not show synergy)
 - High electrode loadings to reduce inactive materials burden

*Beyond Lithium-ion based calculations are supported as part of the Joint Center for Energy Storage Research, an Energy Innovation Hub funded by the U.S. Department of Energy, Office of Science, Basic Energy Sciences.



Sulfur cathodes similar to oxide cathodes in Wh/L and cost if Li and new electrolyte implemented

- Current sulfur batteries use excess electrolyte (10 vs 1 mL/g_s target) to achieve long cycling in DME:DOL
- Cost dominated by Li-metal and inactive materials
 - Benefits only if high loadings can be achieved



Collaboration

- Support EPA in using BatPaC for regulatory analysis
 - Updated the model in response to peer review and state-of-the-art in battery manufacturing and pack design
 - EPA has adopted BatPaC for determining cost of LIB in hybrid and electric vehicle applications
 - Share incremental improvements in BatPaC capabilities
- Project impact of improved components from DOE funded developers (3M, Amprius, Envia)
- Validate design model results with GM model/experience
- Develop and validate NMP recovery process: B&W MEGTEC
- Work with ANL CAMP facility for materials validation & testing

Proposed Future Work

- Study upstream processes and steps in the battery plant to bring greater fidelity in energy and cost estimates
 - Update optimum electrode thickness calculation
 - Complete the cost calculations for the NMP recovery, dry room, and cathode development
 - Update BatPaC cost estimates based on supporting models
 - Include cathode material production processes
 - Explore the energy demands of other steps in the manufacturing process, e.g., electrode coating, formation cycling, etc.
- Include volume expansion mitigation designs (foam or springs, etc)
- Incorporate use of a blended cathode in the model
- Support EPA calculations
- Evaluate fast charging of EV batteries

Summary

- The BatPaC spreadsheet model is a resource for DOE, EPA, and technology developers
 - Projection to the pack level performance helps understand the impact of component technology

Accomplishments

- A new version of BatPaC has been released
 - Another update due in 2015.
- Improved electrode loading sizing calculation
- Translated USABC Pack goals to materials level requirements
- Compared advanced Li-ion to beyond Li-ion Li/S chemistry

Acknowledgements

- David Howell, Peter Faguy, DOE/VTO
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*Beyond Lithium-ion based calculations are supported as part of the Joint Center for Energy Storage Research, an Energy Innovation Hub funded by the U.S. Department of Energy, Office of Science, Basic Energy Sciences.



Technical Backup Slides

Characteristic length for electrolyte transport key to calculating optimal electrode loading

Electrolyte Concentrated Solution
Transport Equation

$$\varepsilon \frac{\partial c}{\partial t} = \frac{\varepsilon}{\tau} \nabla \cdot (D \nabla c) + \frac{\nabla \cdot [(1 - c \bar{V}_e)(1 - t_+^o) \vec{i}_2]}{z_+ \nu_+ F}$$

Electrolyte Characteristic Length,
 L^* , in Porous Electrode

$$L^* = \frac{\left(\frac{\varepsilon}{\tau}\right) D c z_+ \nu_+ F}{(1 - t_+^o) I}$$

Electrode thickness, L , related
to volumetric capacity, Q_v

$$L = \gamma L^*$$

Optimal Loading as a Fraction
of Characteristic Length

$$L = \frac{I t_d}{Q_v}$$

$$Q_A = Q_v L = Q_v \gamma L^* = \sqrt{\frac{\gamma Q_v \left(\frac{\varepsilon}{\tau}\right) D c z_+ \nu_+ F t_d}{(1 - t_+^o)}}$$

$$Q_A [=] \text{ mAh/cm}^2$$

$$Q_v [=] \text{ mAh/cm}^3$$

$$Q_v [\text{ mAh/cm}^3] = \rho \cdot \varepsilon \cdot Q [\text{ g/cm}^3_{\text{act}} \cdot \text{ cm}^3_{\text{act}}/\text{cm}^3_{\text{elect}} \cdot \text{ mAh/g}]$$

Measuring rate capability as a function of electrode loading - towards thick electrodes

- Full-cell, single-layer 14 cm² pouch-cells (NMC622/Graphite)
- Discharge capacity as a function of increasing C-rate
- Thinner electrodes can utilize higher C-rates
- How do we predict the fall off point for thicker electrodes?
- How does one design the highest electrode loading for an expected discharge rate?

